

CLAIMS:

1. A method for characterising the structure or sub-structure of a glycan or glycan derivative, comprising the steps of:
 - experimentally deriving the mass of an unidentified glycan molecule;
 - 5 comparing the mass of the unidentified glycan molecule with defined glycan structures to select candidate structures for the glycan molecule;
 - experimentally deriving the mass of fragments of the glycan molecule;
 - conducting theoretical fragmentation of the selected candidates;
 - matching the mass of the fragments of the unidentified glycan molecule with the
 - 10 mass of fragments theoretically derived from the candidate structures;
 - scoring to produce ranked confidence scores for each of the candidate structures by comparing the masses of the experimentally derived fragments with the masses of the theoretically derived fragments; and
 - if insufficient confidence is obtained in the highest ranked score, further
 - 15 including the step of repeating the process by taking into account more complex cleavage patterns in the theoretical fragmentation step, or by obtaining further fragments.
2. A method as claimed in claim 1 wherein the initial fragment data set used for comparison with the experimentally determined mass consists only of fragments that
- 20 are the result of 1-cleavage fragmentation.
3. A method as claimed in claim 2 wherein the initial fragment data set also include 2-cleavage events which are formed exclusively from glycosidic cleavage types.
4. A method as claimed in any preceding claim wherein scoring is carried out
- 25 using the algorithm
$$\text{Score} = (a - 0.25b) / (m - 1)$$
where a is the number of cleavage points assigned to 1-cleavage events, and b is the number of cleavage points assigned to 2-cleavage fragments.
5. A method as claimed in claim 1 wherein scoring is carried out utilising a
- 30 segmentation scoring method to produce ranked confidence scores for at least one of the candidate structures by counting the number of possible conformations for a glycan identified by a set of matching oligosaccharide fragments and assessing the quality of match for the candidate structure by determining how well a particular conformation is supported by the evidenced fragments

6. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 5 wherein the segmentation scoring method is used for a plurality of the candidate structures.
7. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 5 or 6 wherein the score for ordered segments arising from 1- cleavage fragmentation is calculated to be the number of arrangements for each segment multiplied by the minimum number of points that each segment can attach to the other segment.
8. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in any one of claims 5 to 7 wherein the score is calculated as the number of arrangements of monosaccharides in the segment, multiplied by the number of points that an ordered segment will attach to.
9. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 7 wherein additional information from 2- cleavages that span the boundary between two segments are used to reduce the possible number of positions that the segment can be connected.
10. A method for characterising the structure or sub-structure of a glycan or glycan derivative, comprising the steps of:
- experimentally deriving the mass of an unidentified glycan molecule;
 - 20 comparing the mass of the unidentified glycan molecule with defined structures to select candidate structures for the glycan molecule;
 - experimentally deriving the mass of fragments of the glycan molecule;
 - conducting theoretical fragmentation of the selected candidates;
 - matching the mass of the fragments of the unidentified glycan molecule with the
 - 25 mass of fragments theoretically derived from the candidate structures; and
 - utilising a segmentation scoring method to produce ranked confidence scores for at least one of the candidate structures by counting the number of possible conformations for a glycan identified by a set of matching oligosaccharide fragments and assessing the quality of match for the candidate structure by determining how well
 - 30 a particular conformation is supported by the evidenced fragments.
11. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 10 wherein the segmentation scoring method is used for a plurality of the candidate structures.
12. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 10 or 11 wherein the score for ordered segments arising from 1- cleavage fragmentation is calculated to be the number of arrangements for each
- 35

segment multiplied by the minimum number of points that each segment can attach to in its next segment.

13. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in any one of claims 10 to 12 wherein the score is calculated as the number of arrangements of monosaccharides in the segment, multiplied by the number of points that an ordered segment will attach to.

14. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 13 wherein additional information from 2- cleavages that span the boundary between two segments are used to reduce the possible number of positions that the segment can be connected.

15. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 13 including the step of accounting for uneven sub-segment size and multiple independent cleavage events.

16. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in any one of claims 10 to 15 wherein redundant fragments and, when known, chemically impossible fragmentations are omitted to reduce the amount of fragments and data to be processed.

17. A method for characterising the structure or sub-structure of a glycan or glycan derivative as claimed in claim 14 wherein the score is calculated using the equation:

$$\text{score}(\text{segment}) = \frac{\text{arrangements}(\text{subsegments}) \times \prod_{s \in \text{subsegments}} \text{score}(s) \times \text{number of attachment points}}{\text{number of anchoring segments}}$$